

(1,3-¹³C₂)Propan-2-ol
117072-72-7 | DTXSID90745872

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 23.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.91e-01

Confidence level: 7.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methoxyamine</div> <div>Measured: 45.4</div> <div>Predicted: 217</div>	<div>Image not found</div> <div>Salicylic acid</div> <div>Measured: 21.0</div> <div>Predicted: 2.08e-05</div>	<div>Image not found</div> <div>Barbituric acid</div> <div>Measured: 6.70</div> <div>Predicted: 4.85e-08</div>
<div>Image not found</div> <div>Isobutylamine</div> <div>Measured: 10.4</div> <div>Predicted: 172</div>	<div>Image not found</div> <div>2-Chloropropan-1-ol</div> <div>Measured: 18.3</div> <div>Predicted: 4.93</div>	